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Simulation of heavy ion beams with a semi-Lagrangian Vlasov solver

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Abstract

We introduce the semi-Lagrangian Vlasov method, which computes the distribution function of the particles on a grid in phase space, to beam propagation in a uniform focusing channel. With this new tool, we study halo formation in a mismatched thermal beam, and the evolution of an initial semi-Gaussian beam. For the latter problem comparisons are made with the Particle-In-Cell code WARP.

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1. Introduction

Particle-In-Cell (PIC) methods have proven very efficient for the simulation of charged particle beams, providing us a better understanding of their behavior, and thus have become indispensable for the design of several kinds of devices. The main advantage of such methods is that they give sufficiently accurate results for the low-order moments of primary interest in beam transport with a fairly small number of particles, and thus make it possible to follow a particle beam for a long time even in a three-dimensional geometry. However in some cases one is interested in more detailed collective wave phenomena, which may occur over shorter time scales. Then the noise inherent in the PIC method can make it difficult to get an accurate description of the phenomenon. Moreover, this noise decreases only as $\sqrt{N}$ when the number of particles N is increased, which makes it inefficient to mitigate noise effects by adding more particles. One option is to employ a perturbative method, such as the δf method [1]. When the distribution changes significantly over time and no clear equilibrium exists, it may be more effective to use a Vlasov solver which discretizes the full phase space on a multi-dimensional grid. Outside of roundoff error

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associated with the numerical operations, this procedure is intrinsically devoid of statistical noise. Errors in this method are associated with discretization of the Vlasov equation on the phase-space grid, as well as truncation errors in the numerical computation of phase-space characteristics. Vlasov methods have proved efficient for several plasma physics problems with intense self-fields [2–5]. Such problems are similar to those associated with the simulation of charged particle beams that are well described by the evolution of a continuous Vlasov distribution.

We investigate here, in particular, the initial evolution of a semi-Gaussian beam for which space charge waves have been observed with the PIC code WARP [6], and also halo formation in a slightly perturbed Maxwell–Boltzmann thermal beam propagating in a uniform focusing channel. Comparisons will be made with WARP in order to evaluate the strengths and weaknesses of both methods. In any case, as the numerical methods are completely different, numerical artifacts in the results should be more easily evaluated by comparing the results obtained with the two methods.

This paper is organized as follows: First, we briefly review the semi-Lagrangian method. Then we observe the formation of a halo in a perturbed Maxwell–Boltzmann beam. After that, we investigate the evolution of an initially semi-Gaussian beam propagating in a uniform focusing channel and we compare the results obtained to those given by the WARP PIC code.

2. The semi-Lagrangian method for an electrostatic Vlasov equation

The principle of the semi-Lagrangian method is to update the value of the distribution function f on grid in phase space for a given species of particles using the property that f is constant along the characteristics. There are two steps in this method: (1) Find for each grid point the origin (at ate previous time step) of the characteristic ending at that grid point, (2) interpolate the value of f at that origin to get the new value of f at the grid point. We refer the reader to Ref. [5] for more details.

In the case of the 2D electrostatic Vlasov equation, a time splitting procedure can be used, whereby the following two equations are solved successively:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_x f = 0 \tag{1}$$

and

$$\frac{\partial f}{\partial t} + (\mathbf{E}_{\mathrm{self}}(\mathbf{x}, t) + \mathbf{E}_{\mathrm{applied}}(\mathbf{x}, t)) \cdot \nabla_v f = 0 \tag{2}$$

By employing a finite difference in time to solve Eqs. (1) and (2) the origin of the characteristics can be computed explicitly. The displacement from the mesh points is the same everywhere, namely $v\Delta t$ for the advection Eq. (1) over a time step Δt and $E\Delta t$ for the advection Eq. (2) over Δt. Only the second step of the algorithm involves effective computation: The distribution function at the previous time step is interpolated by cubic splines (a two-dimensional tensor product of cubic B-splines in each case). This procedure is identical to the one introduced by Cheng and Knorr [7]. Most recently, we have investigated the use of local Hermite interpolation; this works well and might be more suited to massively parallel computation.

3. Halo formation in a mismatched thermal beam propagating in a uniform focusing channel

Heavy ion fusion, as well as other applications, requires drivers capable of accelerating beams to very high energy with minimal particle losses. For this reason it is essential to have a good understanding of halo formation, in particular the mechanisms leading to it and the number of particles involved. Particle-Core models have been able to provide a good description of the amplitude of the halo; however, these are approximate models which do not include the full nonlinear dynamics and cannot predict the number of particles entering the halo that may subsequently be lost. On the other hand, standard PIC codes have, unless a very large number of particles is used, noise levels far too high to give an accurate description of the low densities involved in the halo region. The semi-Lagrangian Vlasov method, which is completely devoid of statistical particle noise and resolves the low-density halo region as well as the high-density core region, is able to provide new insights into the dynamics of halo formation. Another advantage is that the method makes it convenient to simulate pure modes, which is very hard in PIC codes because the particle noise necessarily excites a spectrum of modes.

Starting from an axisymmetric thermal beam in a Maxwell–Boltzmann transverse equilibrium, we perturbed the density by 50%, using 1.5 times the equilibrium density (corresponding to a radial mismatch of approximately 25%). This triggers the so-called breathing mode which expels particles into the halo. The parameter of our runs were as follows: particle species: singly ionized potassium ($Z = 1$, $m = 39.1\,\mathrm{amu}$), beam energy $8 \times 10^4\,\mathrm{eV}$, current 0.2 A, beam radius 1 cm (rms edge measure).

In the simulations presented we adjusted the applied focusing field for a tune depression of $\sigma/\sigma_0 = 0.5$. Here σ and σ_0 denote the phase advance of the particles in the presence and absence of charge. Note that a Maxwell–Boltzmann equilibrium can be obtained at different tune depressions by varying the temperature; see Ref. [8]. For these parameters we plotted the projection of the distribution function onto the x–y and x–v_x planes, as well as a slice of the decimal logarithm of the density in the mid-plane ($y = 0$) at different values of z. All the values of z were chosen numerically to correspond to the same phase in the

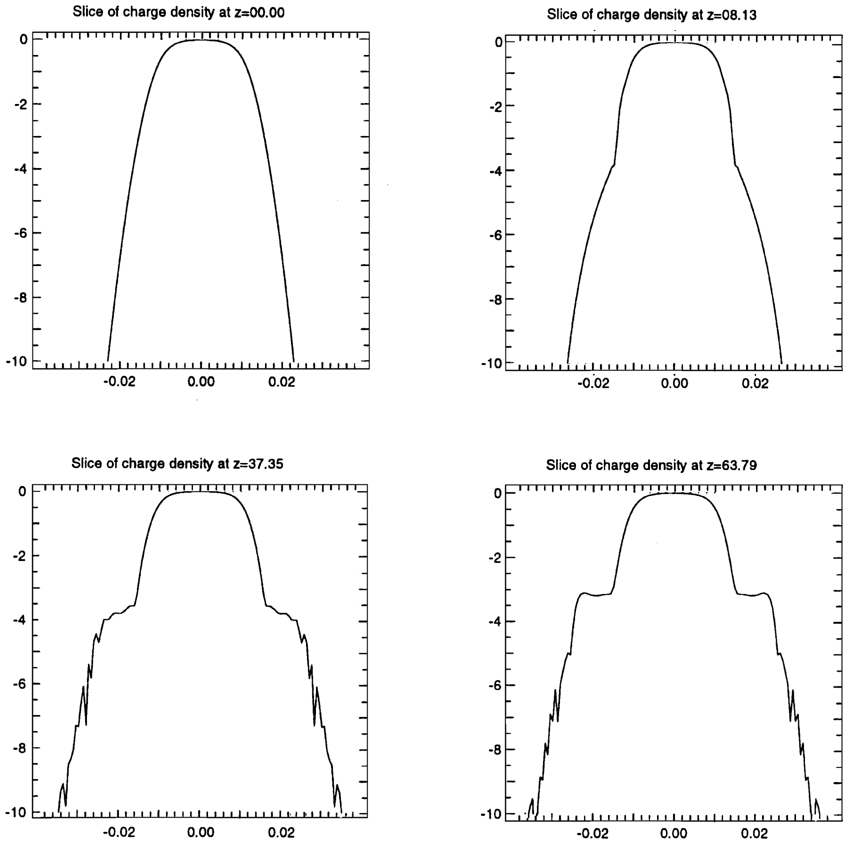

Fig. 1. Halo formation: slice of charge density at $y = 0$ for Vlasov simulation at initial and 3 later times.

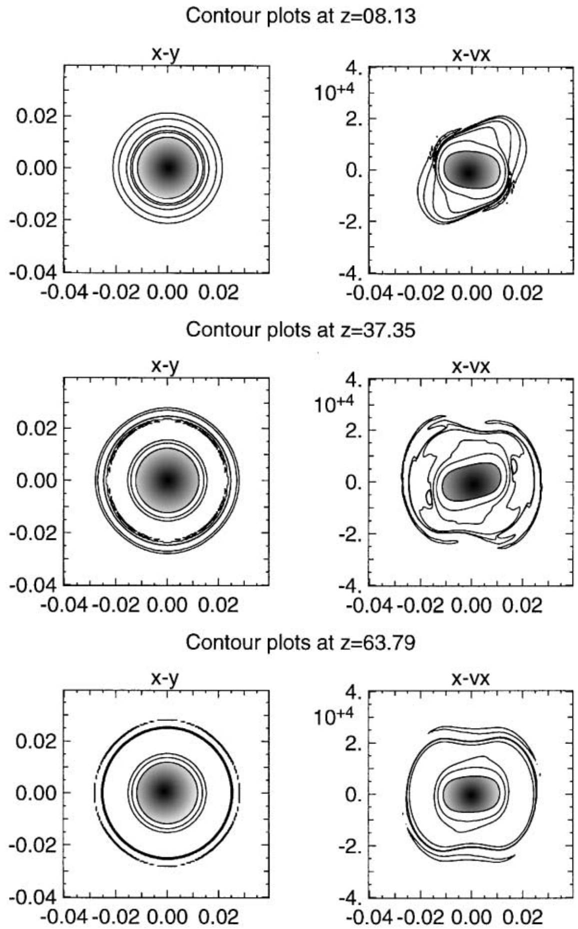

Fig. 2. Halo formation: contour plots of phase-space projections for Vlasov simulation at three times.

breathing mode oscillation, which was chosen to be close to the maximum point in $\mathrm{d}x_{\mathrm{rms}}/\mathrm{d}z$. In order to emphasize the halo, we added to the linearly scaled standard shaded contour values, isolines corresponding to values of 0.1, 0.01, 0.001, 0.0001 and 0.00001 of the maximum value of the distribution function.

We see, in the slice plots (Fig. 1) and in the phase-space contour plots (Fig. 2), a well-defined halo, which corresponds to a plateau in the slice plot at roughly 1/1000 of the maximum value of the density. Beyond the edge of this plateau there is a sharp drop of the density, which suggests that very few particles go further out. It is thus natural to define the edge of the halo to be the edge of this plateau. As evident from the phase-space plots, this halo is also the usual envelope particle resonant surface seen in core-particle simulations [9]. For our beam, whose core has a 1 cm radius, the edge of this plateau is at approximately 2.6 cm. Using Wangler's empirical formula [9], we should get a maximum radius for the particles of 2.41 cm, which is close to our value. In any case, our first results with the semi-Lagrangian Vlasov code look very promising. More comparisons need to be made, and numerical studies are in progress.

4. Evolution of a semi-Gaussian beam in a uniform focusing channel

4.1. Vlasov simulation

Our aim here is to study the evolution of a rms-matched initial semi-Gaussian beam in a uniform focusing channel. The initial semi-Gaussian has uniform density and Gaussian fall off in velocity space. Such an initial condition is not an equilibrium of the focusing channel and will evolve.

In the run shown, the beam particles are singly ionized potassium ($Z = 1$, $m = 39.1\,\mathrm{amu}$), the beam kinetic energy is 80, 000 eV, its current is 0.2 A, and its radius is 2 cm. The tune depression is $\sigma/\sigma_0 = 0.25$. The beam is moving in a round conducting pipe of radius 3 cm. A grid of 64^4 nodes was employed to represent the (x, y, v_x, v_y) phase space.

Slice plots of the density for different values of z are given in Fig. 3. We notice that the beam at first becomes hollow, then the regions of high density propagate to the core of the beam and out again, via space charge waves. These waves disperse and are damped by phase mixing after a few lattice periods. The results we present in the slice plots go up to 3 lattice periods. However, longer runs have been performed and the oscillations damp rapidly until they are almost nonexistent after roughly 10 lattice periods, by which time an equilibrium appears to have been reached. These results are consistent with WARP PIC simulations presented by the Maryland group on their beam propagation experiment [6].

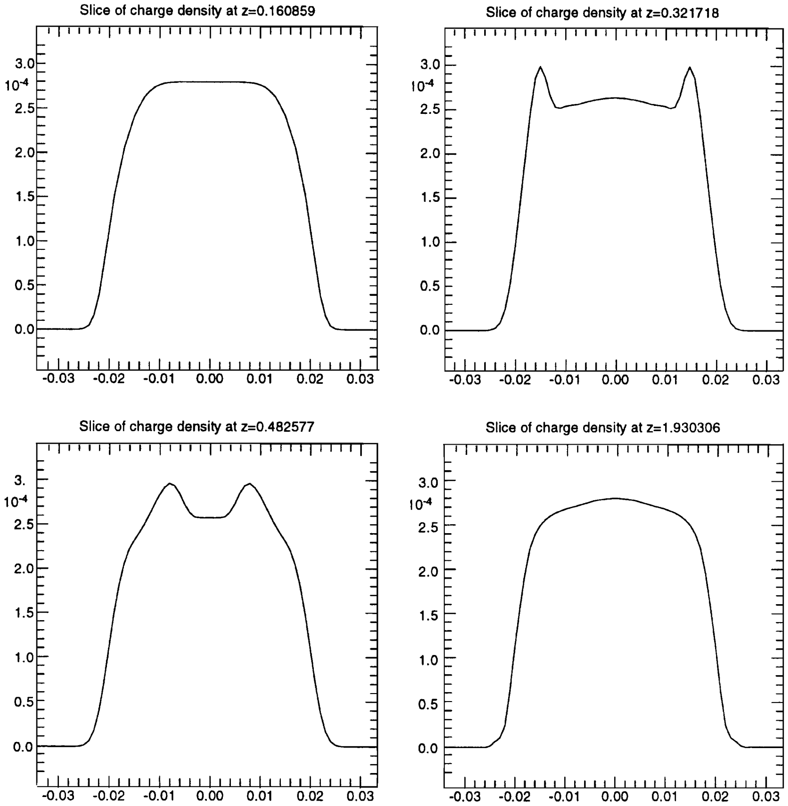

Fig. 3. Initial semi-Gaussian beam at $y=0$ integrated over p_x and p_y, for Vlasov simulation at 4 times.

4.2. Comparison with WARP

In Fig. 4, slice plots of the charge density after $z = 0.4826$ m for a series of WARP PIC runs with increasing number of particles are given. On all the plots the dashed curve represents the semi-Lagrangian Vlasov solution. For the grid used, the simulation time used by the semi-Lagrangian Vlasov code is roughly equivalent to that of WARP when the latter is running with 5 million particles; both codes were run on 32 processors of NERSC's T3E. We notice on these plots how the noise is reduced when the number of particles is increased; with 20 million particles the WARP solution is very close to the Vlasov solution. However, we notice that even with 20 million particles there is still a little bit of noise, which prevents WARP from following the oscillations longer in time as they become damped in amplitude. On the other hand, even with 50,000 particles (for which WARP is much faster than the Vlasov code) the charge density waves can be observed at the beginning, even though they are quickly lost in the noise. A time-averaged diagnostic would make the PIC data cleaner, but subtle features are soon lost nonetheless.

5. Conclusion

Even though the Particle-In-Cell method can be expected to remain the method of choice for full scale driver simulations, the semi-Lagrangian Vlasov method is proving to be a useful tool for some specific problems, such as the study of space

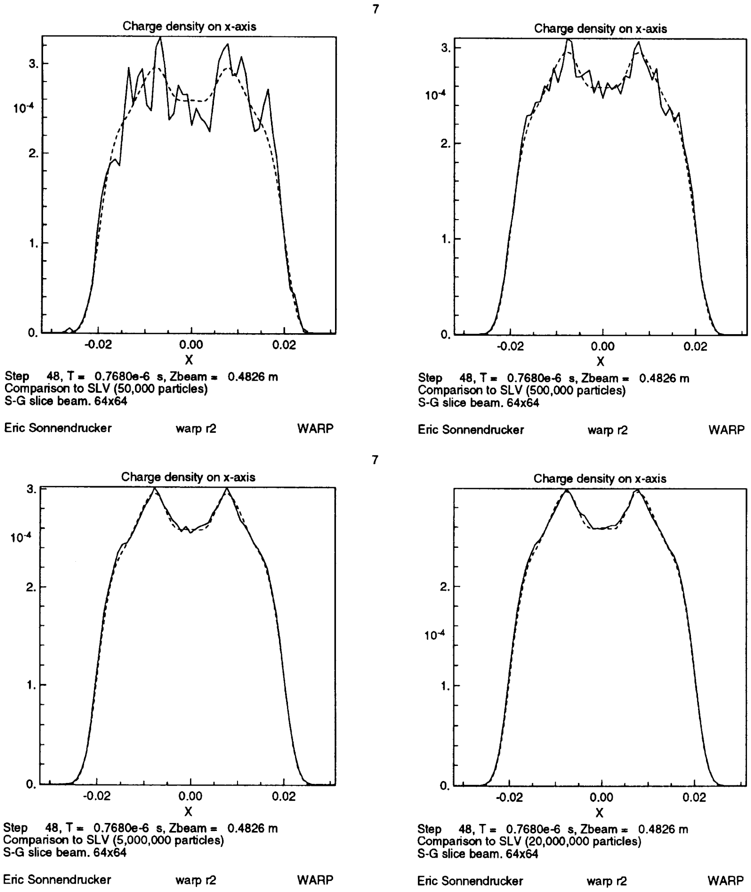

Fig. 4. Comparison of WARP with semi-Lagrangian Vlasov simulation of initial semi-Gaussian beam, after 0.4826 m (slice of charge density for 50 K, 500 K, 5 M and 20 M particles).

charge waves on an initial semi-Gaussian beam, and especially halo simulations for which the low-density regions of phase space need to be well resolved. Its main asset is that it is devoid of statistical particle noise and therefore can give information on details that can be obscured by the noise in particle simulations. Furthermore, since the numerical method is very different, comparisons with PIC calculations can help in separating numerical artifacts from physics. The main limitations of the method are the large amount of computer memory needed for implementation which can be mitigated by appropriate meshing schemes.

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